CSP
Grupo de Investigación en Control y Supervisión de Procesos

Universidad de Valladolid

InCO4In

Integrated plant-wide control and optimization for industry4.0

bio2eng
BIOSYSTEMS & BIOPROCESS ENGINEERING

CSIC
Consejo Superior de Investigaciones Científicas

Simulación Predictiva de la red de H_2 de una Refinería de Petróleo

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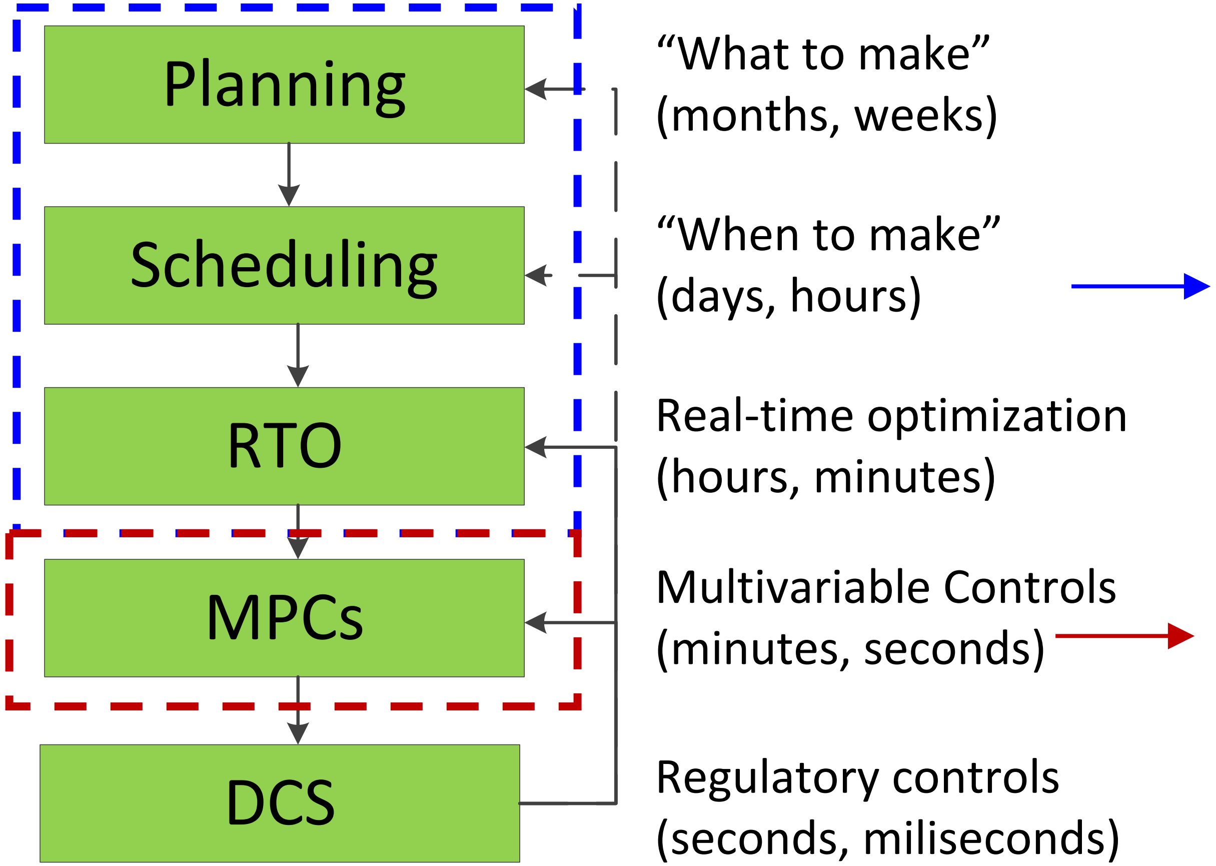
Workshop final
20-21 junio, 2022

DECISION-MAKING PROCESS IN MANUFACTURING OPERATIONS



Steady state models with multiple process units in scope: MINLP, MILP and/or NLP

Dynamic state models with single process units in scope: LP, QP or NLP.

Hydrogen in petrol refineries

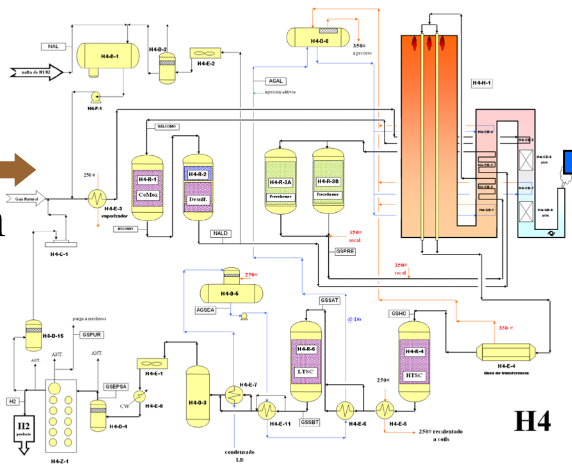
Hydrogen is used in modern refineries in processes that have two main purposes:

- ✓ Increase the value of the hydrocarbons (platformers, hydrocraking, etc.)
- ✓ Reduce the sulphur content of the products, (HDS),..

Hydrogen plants (producers/consumers)

HC

Steam



H_2

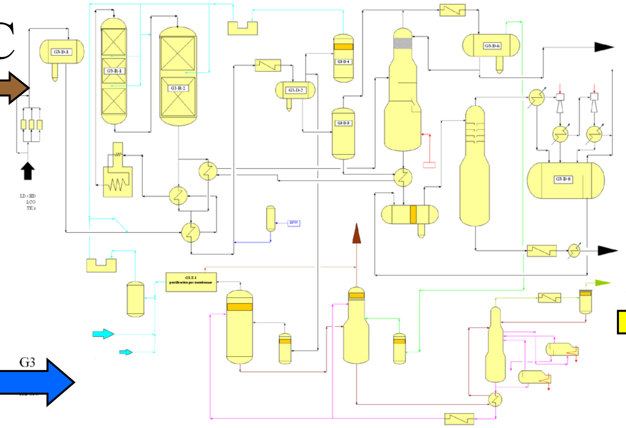
Flow

Purity

Hydrogen producer plant

catalytic hydrotreating reactions

HC



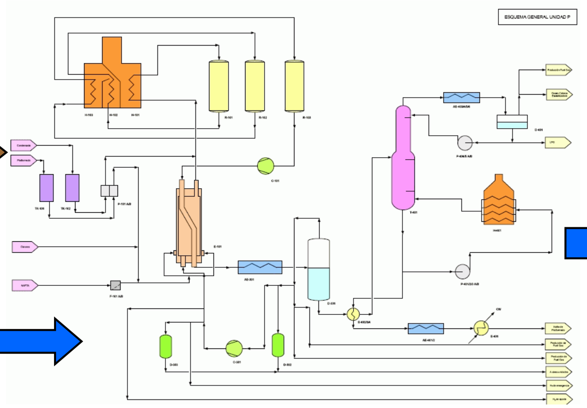
S

H_2

Hydrodesulphurization plant HDS

Hydrocrakers

HC



H_2

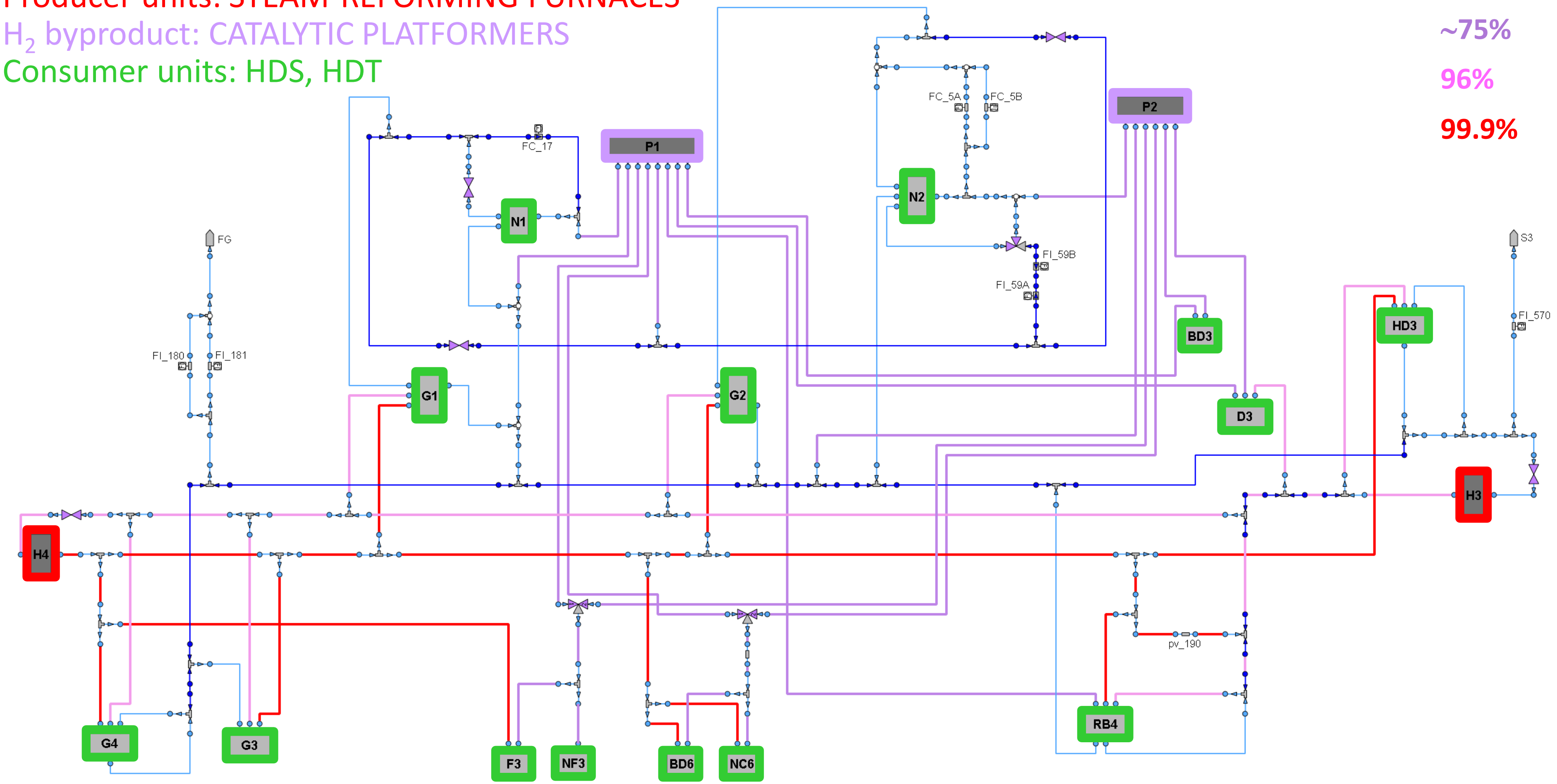
Low purity H_2 obtained as a by-product

Platformer

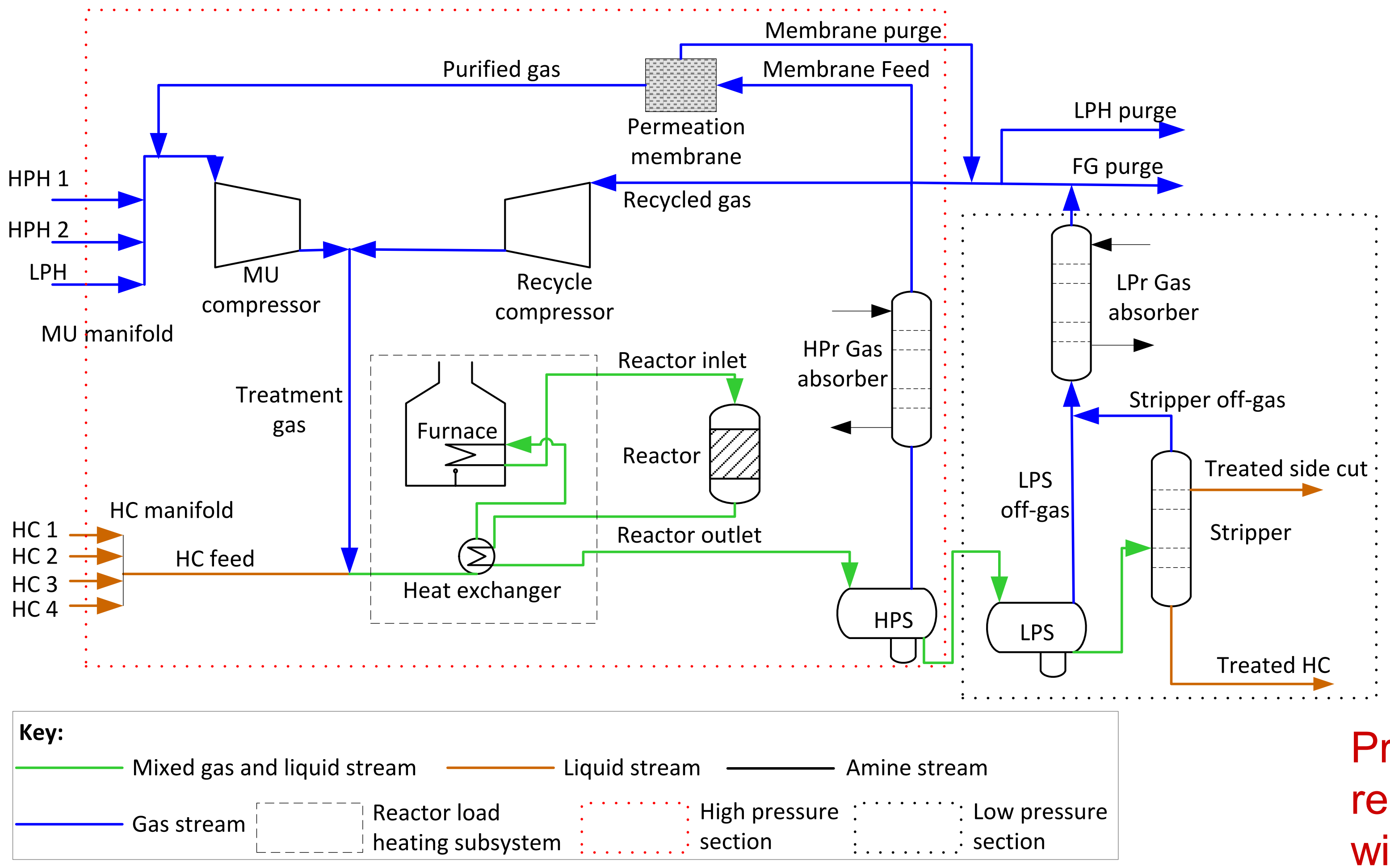
Producer units: STEAM-REFORMING FURNACES

H_2 byproduct: CATALYTIC PLATFORMERS

Consumer units: HDS, HDT



Simplified schematic

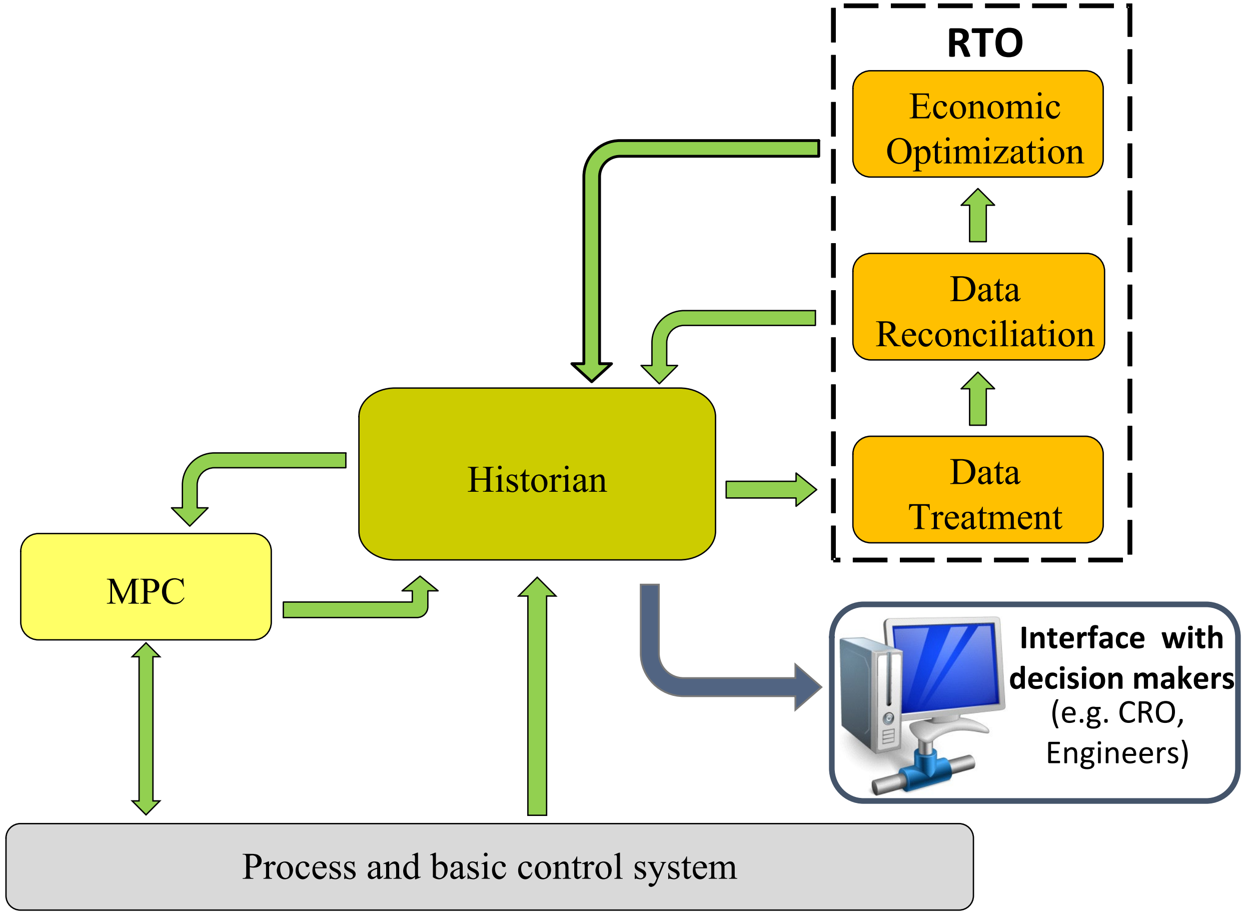


Variable hydrogen demand according to the type and flow of the hydrocarbon being treated

The excess hydrogen is partly recycled, partly sent to the fuel-gas FG or CBP networks to prevent accumulation of impurities

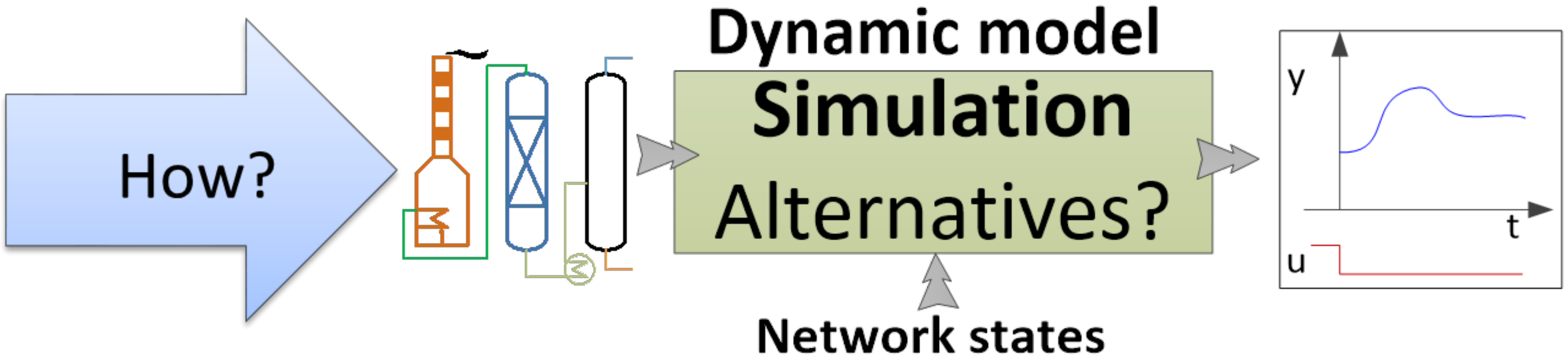
Preserving catalyst life requires to operate always with excess hydrogen in the reactors

Current Hydrogen Network Control Architecture



- RTO implementation led to improvements in H_2 network management strategies (e.g. purification units use)
- Better understanding of impacts of changes across the network

RTO: Real-time optimization.
MHE: Moving horizon estimation.
MPC: Model predictive control.
CRO: Control room operators.


How?
Dynamic model
Simulation
Alternatives?
Network states
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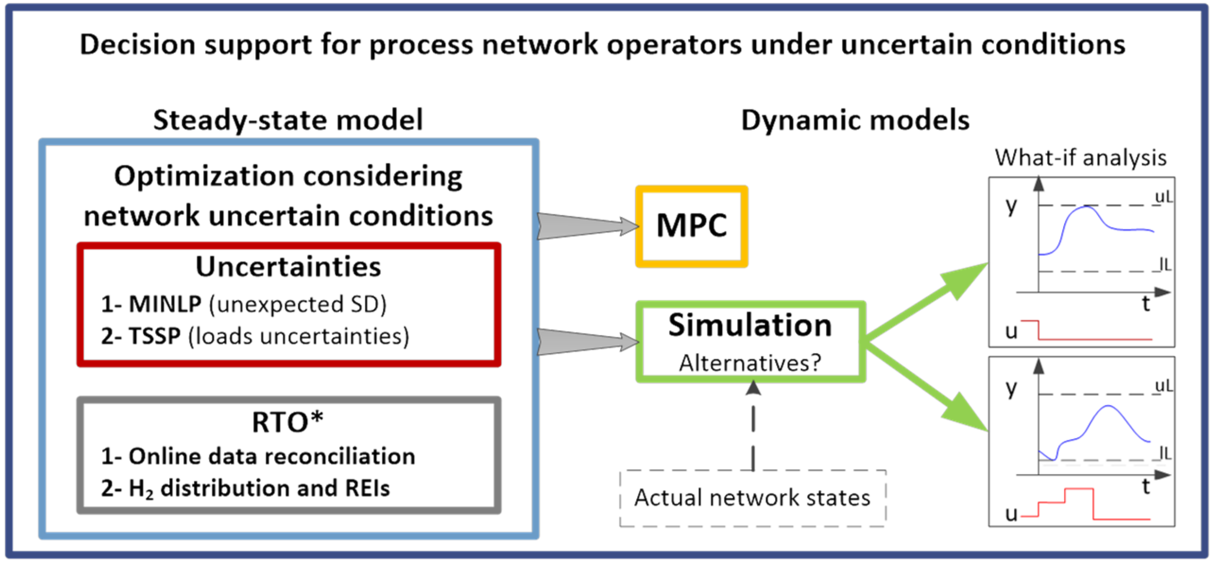


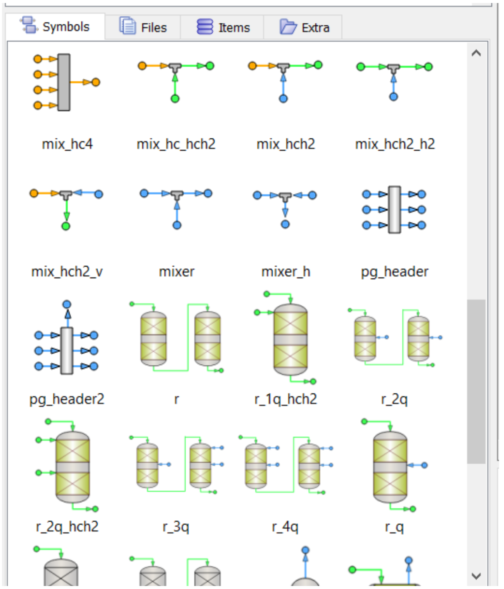
- Develop tools that fit together smoothly
- Enable decision-making at process unit and plant level
- Account for uncertainties
- Expand operator's visibility w.r.t. process change of conditions

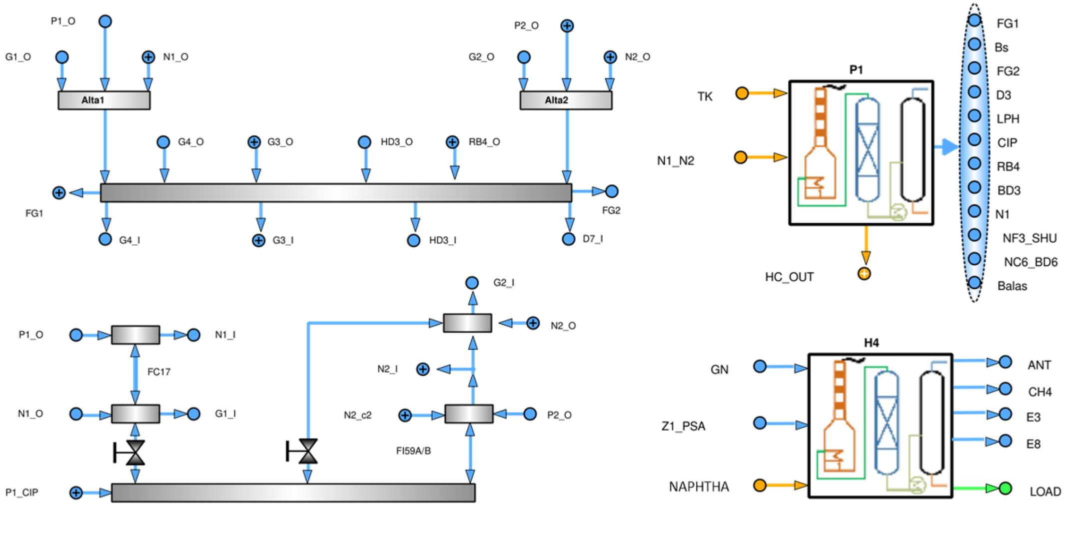
Objective

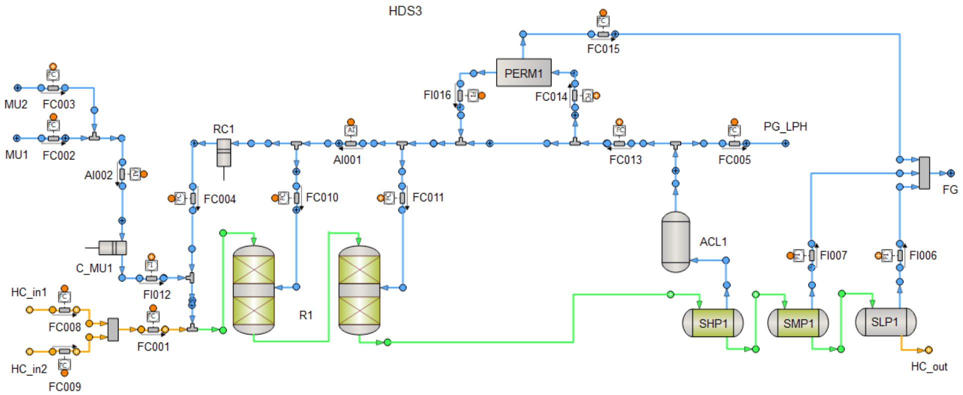
Develop a comprehensive first-principles based library, capable of:

- representing an actual process network,
- its dynamics for a hydrogen network case study, and
- run with real-time data inputs and offline data.

Proosis / EcoSimPro®[1]

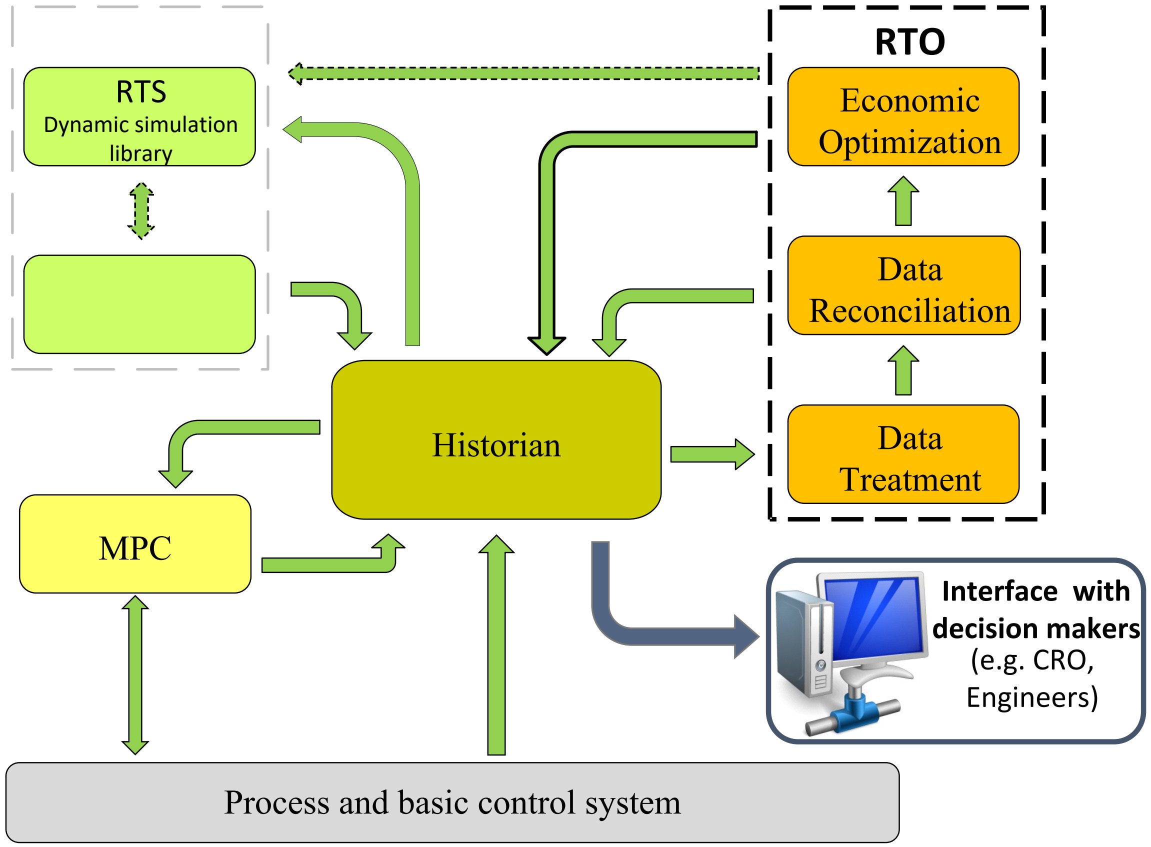






Implementation in real-time environment

- Use in a decision support framework structure



RTS: Real-time simulation.
RTO: Real-time optimization.
MHE: Moving horizon estimation.
MPC: Model predictive control.
CRO: Control room operators.

MHE formulation

Given:

- H_2 network dynamic nonlinear model (1,2)
- Plant measurements (e.g.: HC loads, gas purity / flowrates; 3)
- Previous manipulated variables values (3)
- Presence of disturbances (*w*, 1, 4)

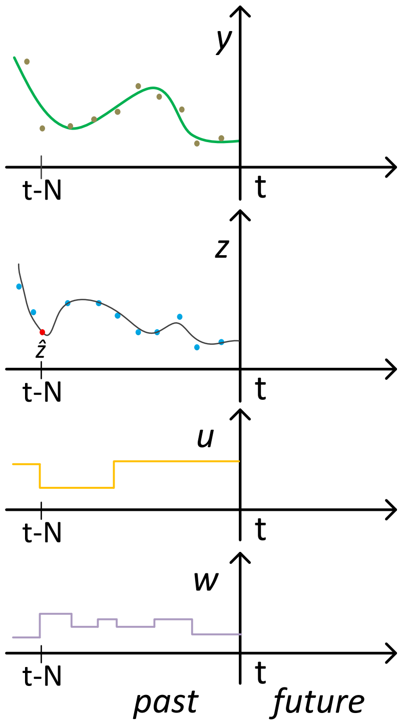
$$f(z(t), \dot{z}(t), u(t), p, w(t)) = 0, \qquad z(0) = z_0, \quad (1)$$

$$y_m(t) = h(z(t), u(t), p), \quad (2)$$

$$I^{(N)}{}_k \triangleq col(y_{k-N}, \dots, y_k, u_{k-N}, \dots, u_{k-1}), \quad (3)$$

$$\Delta w_k = w(k) - w(k-1), \quad (4)$$

$$k = 1, 2, \dots, N$$



MHE formulation

Solve:

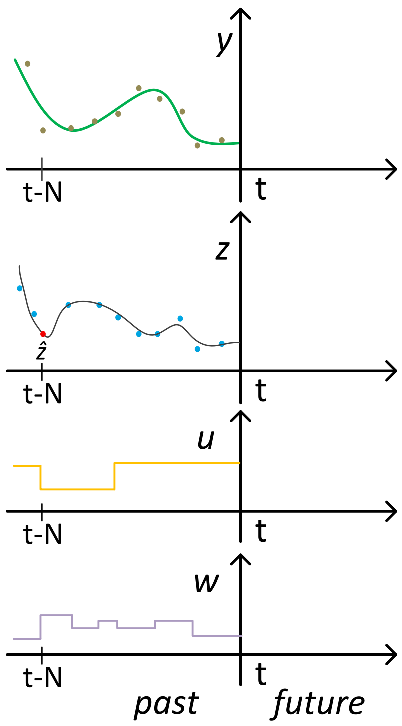
$$\min_{\left(\hat{z}_{t-N}, w_{k-N}, \cdots w_k, \hat{p}\right)} \left\{ \left\| \hat{z}_{t-N|t} - \bar{z}_{t-N} \right\|^2_P + \sum_{i=k-N}^{k} \left\| \Delta w_{k-i} \right\|^2_Q + \sum_{i=k-N}^{k} \left\| y_i - y_m(i) \right\|^2_R \right\} \quad (5)$$

s.t.

$$z_{lb} \leq \hat{z}_k \leq z_{ub}$$

$$y_{lb} \leq y_m \leq y_{ub}$$

$$w_{lb} \leq w_k \leq w_{ub}$$



Then the DAEs for initial time *t-N* to current time *t* to find current state z_t is solved

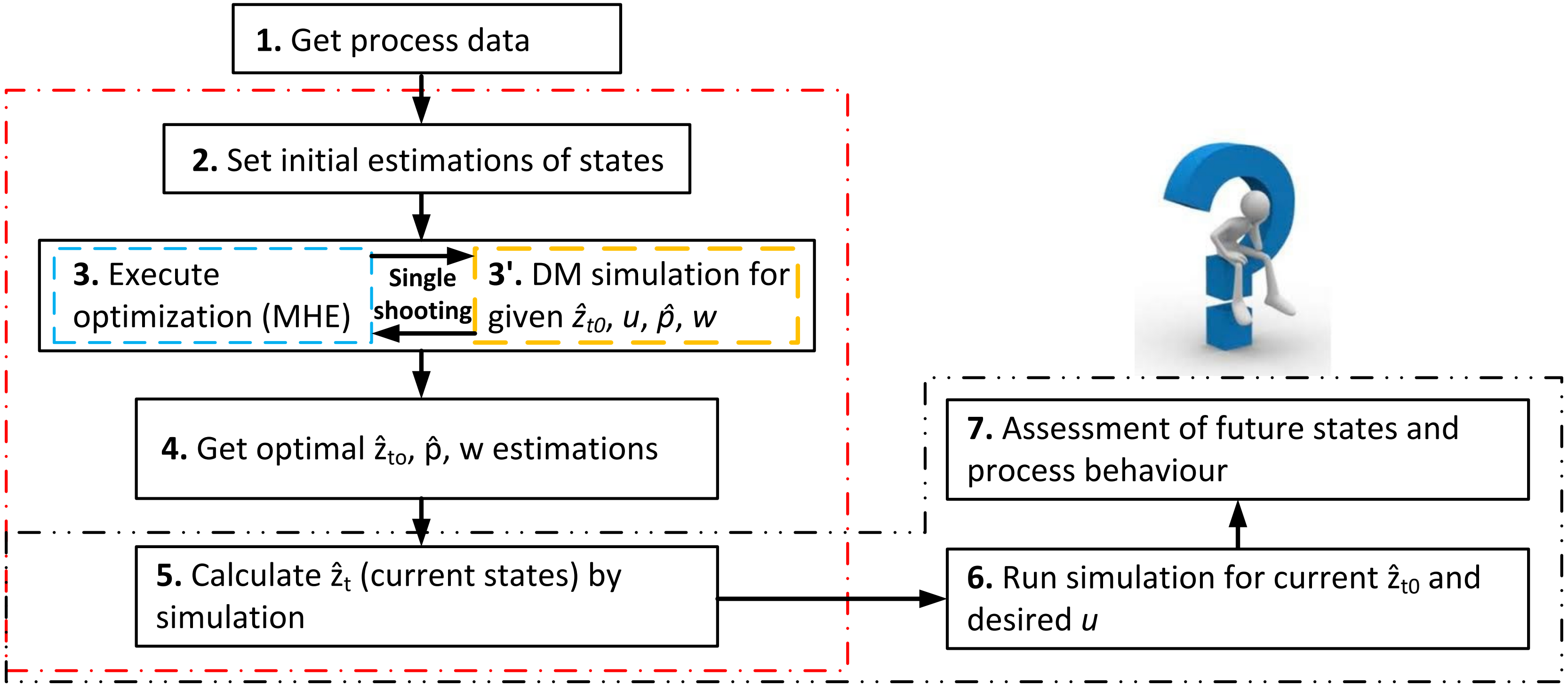
Using: $\hat{p}, \hat{w}_k$

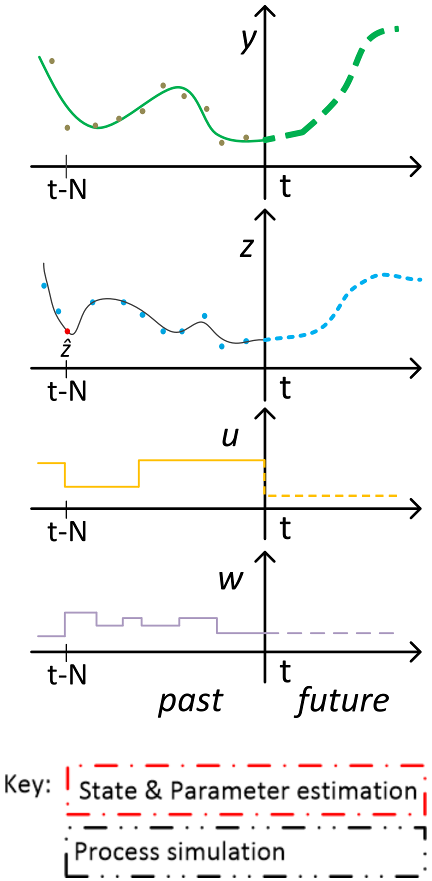
$$f(z, \dot{z}, u, p, w, t) = 0$$

$$z(t-N) = \hat{z}_{t-N}$$

MHE and simulation integration

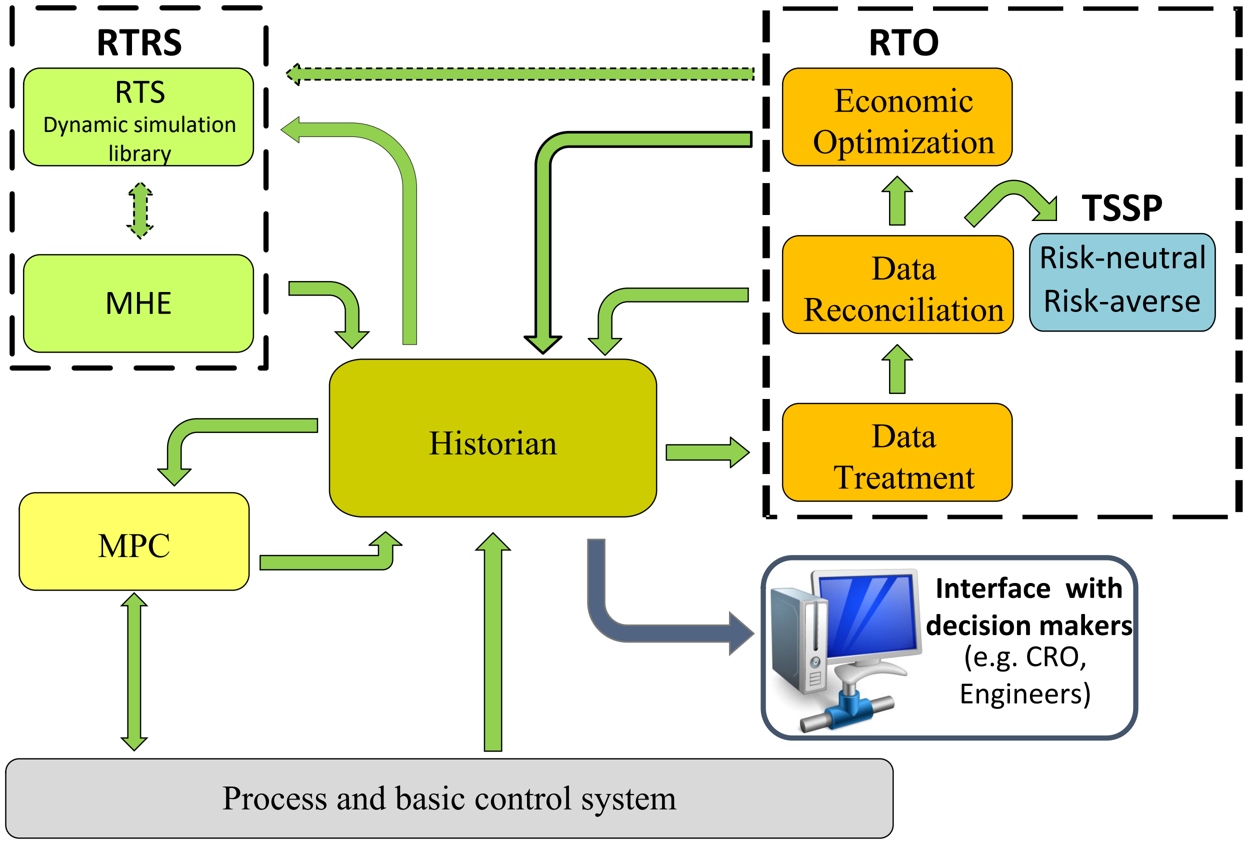
Roadmap implemented on Proosis / EcoSimPro®[1]





Implementation in real-time environment

Use in a decision support framework structure



TSSP: Two-stage stochastic programming.
RTRS: Real-time reconciled simulation.
RTS: Real-time simulation.
RTO: Real-time optimization.
MHE: Moving horizon estimation.
MPC: Model predictive control.
CRO: Control room operators.

Case study

- H_2 network (simplified)
- 2 producers and 3 consumers
- Analyse RTRS value as decision support tool

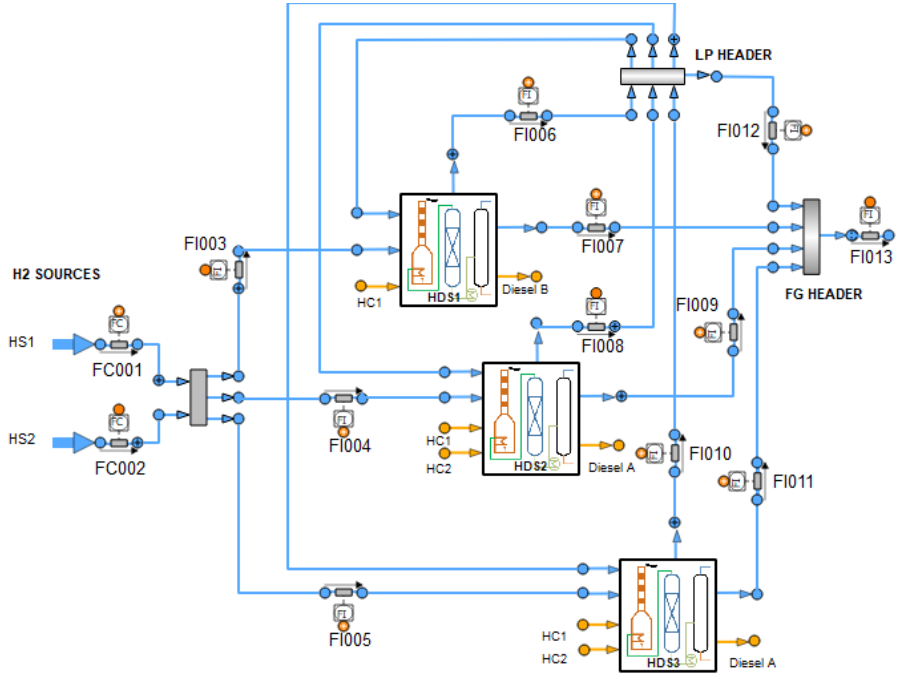


Table 2.1. Summary of characteristics of the model

INFO	VALUE
Number of equations	1279
Number of boxes (coupled subsystems of equations)	5
Number of input DATA	590
Number of input BOUNDARIES	13
Number of output EXPLICIT	1247
Number of output DYNAMICS or DERIVATIVES	27
Number of output ALGEBRAICS	5
Size of Jacobian matrix (DYNAMIC+ALGEBRAIC).	32x32
Default integration method	DASSL

PC Intel® Core™ i7-6500U CPU @2.50 GHz RAM 16 GB, and takes on average 40s per sample time.

Case study

- 15 Manipulated variables (N = 5)
- Scenario-based analysis (What-if)

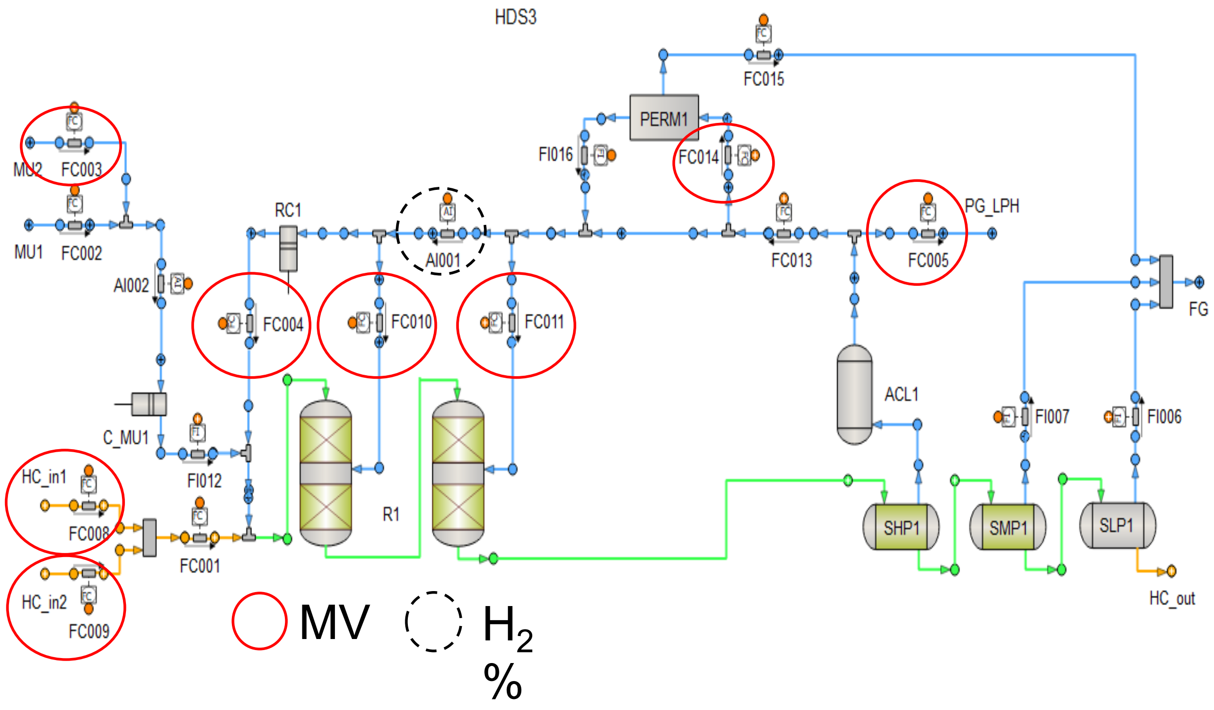
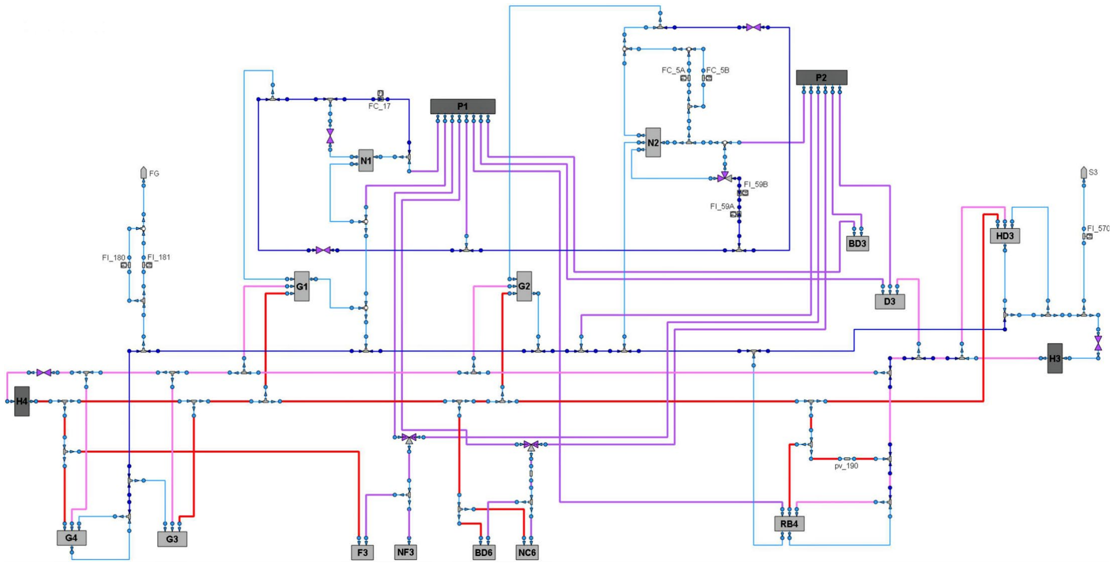
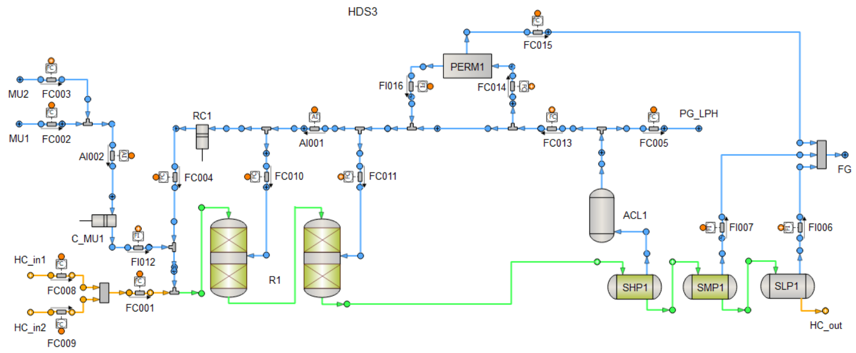


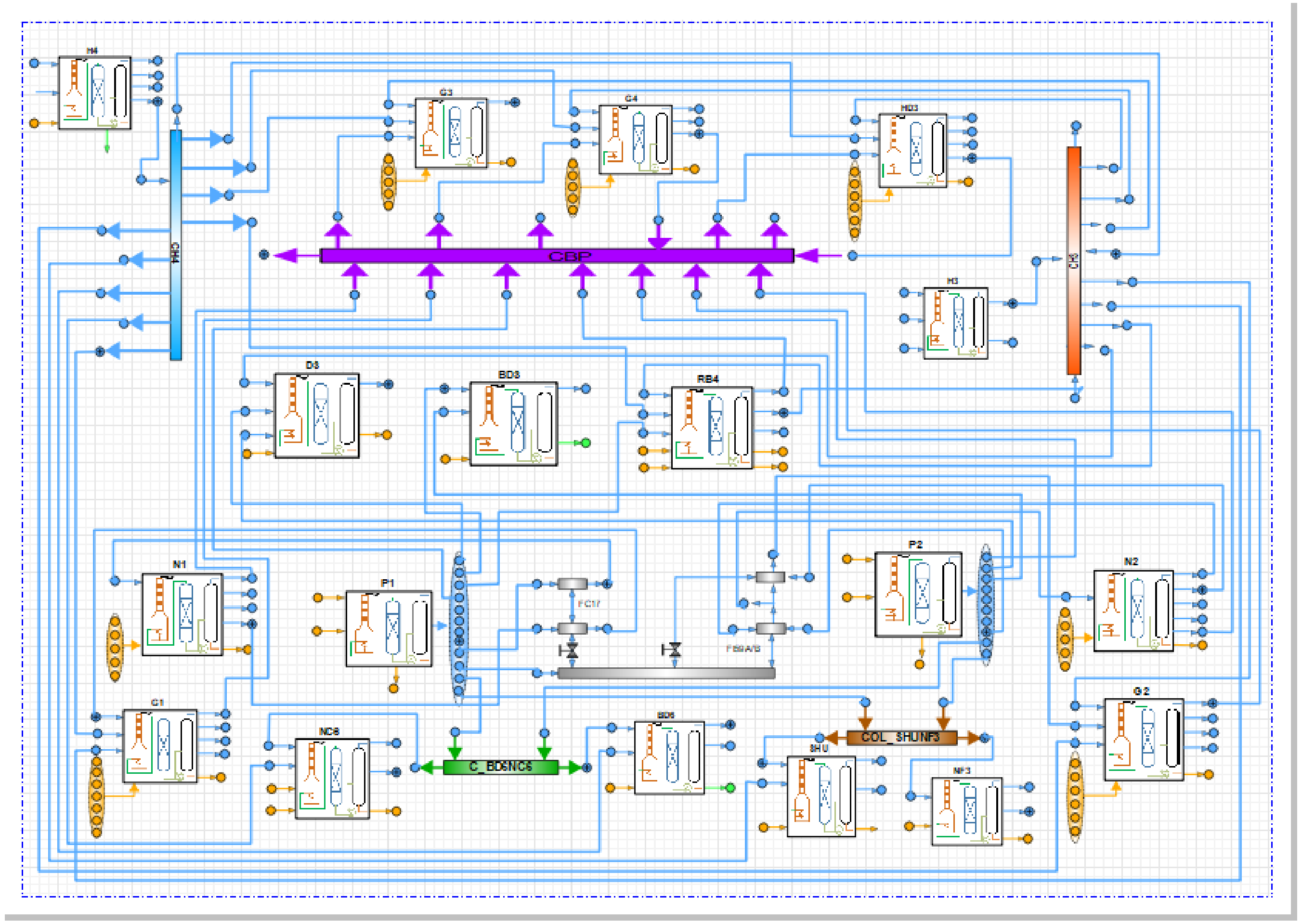
Table 2.2. Summary of manipulated variables of each HDS in the model.

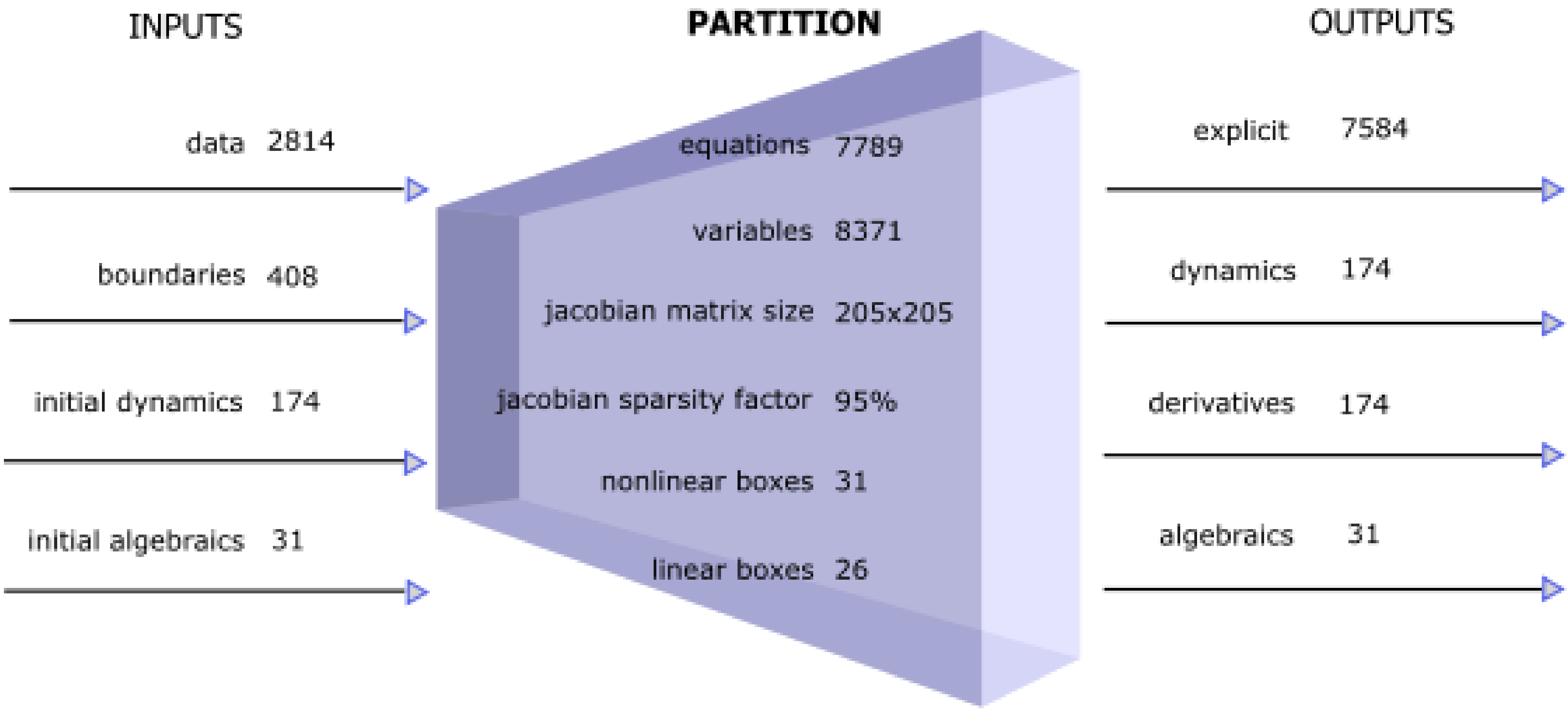
	HDS1	HDS2	HDS3
FC001	MV1		
FC002	MV2		
FC003		MV1	MV1
FC004	MV3	MV2	MV2
FC005	MV4	MV3	MV3
FC008		MV4	MV4
FC009		MV5	MV5
FC014			MV6

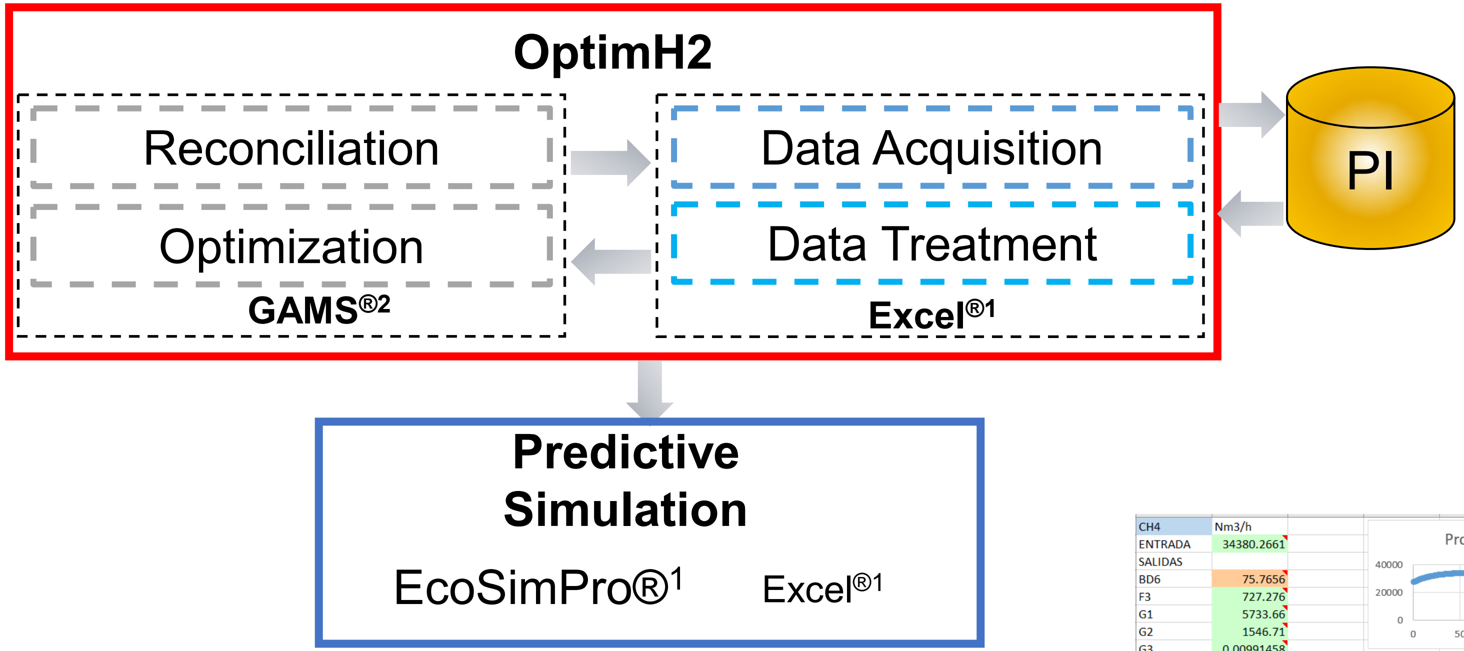
Predictive Simulation

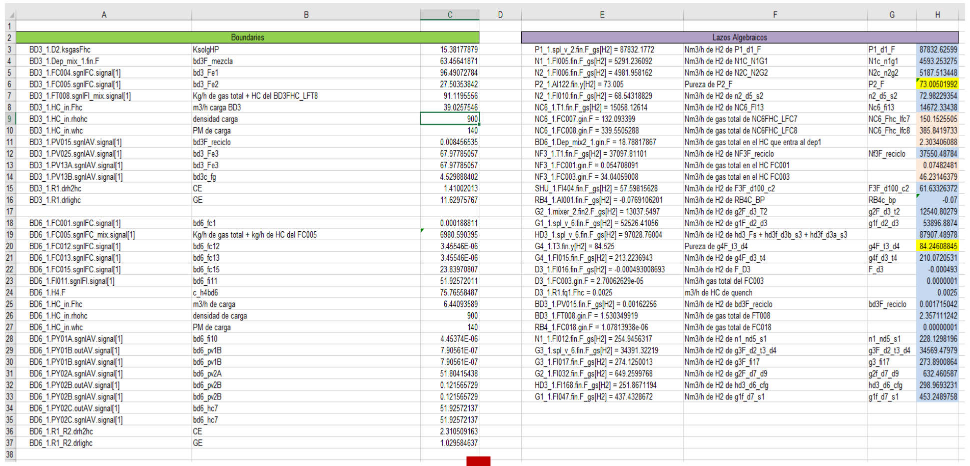


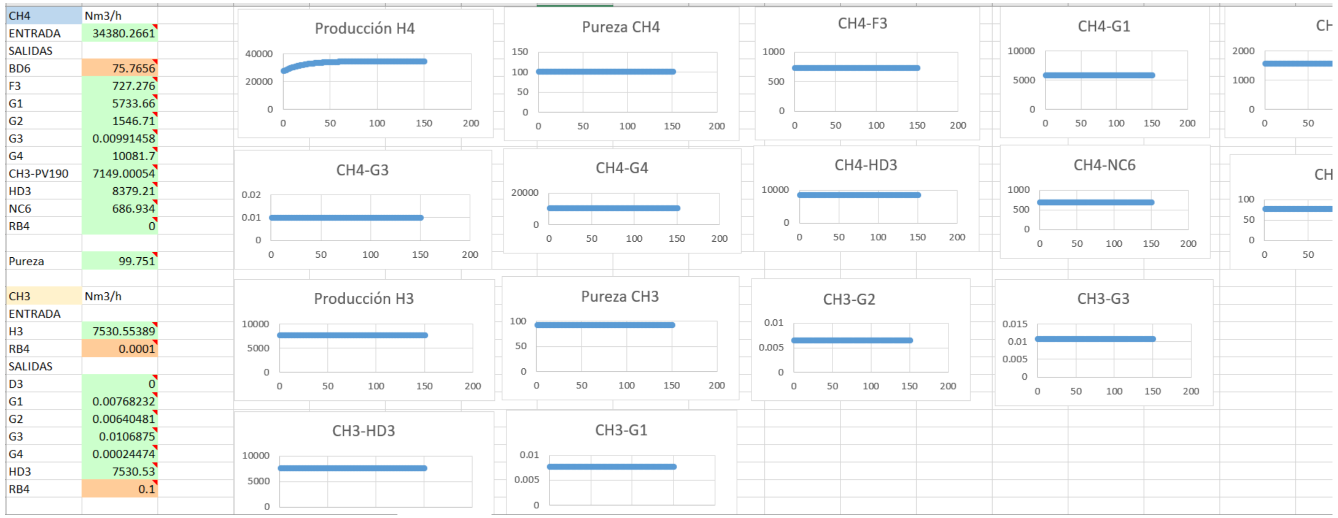





INPUTS
PARTITION
OUTPUTS
data 2814
boundaries 408
initial dynamics 174
initial algebraics 31
equations 7789
variables 8371
jacobian matrix size 205x205
jacobian sparsity factor 95%
nonlinear boxes 31
linear boxes 26
explicit 7584
dynamics 174
derivatives 174
algebraics 31





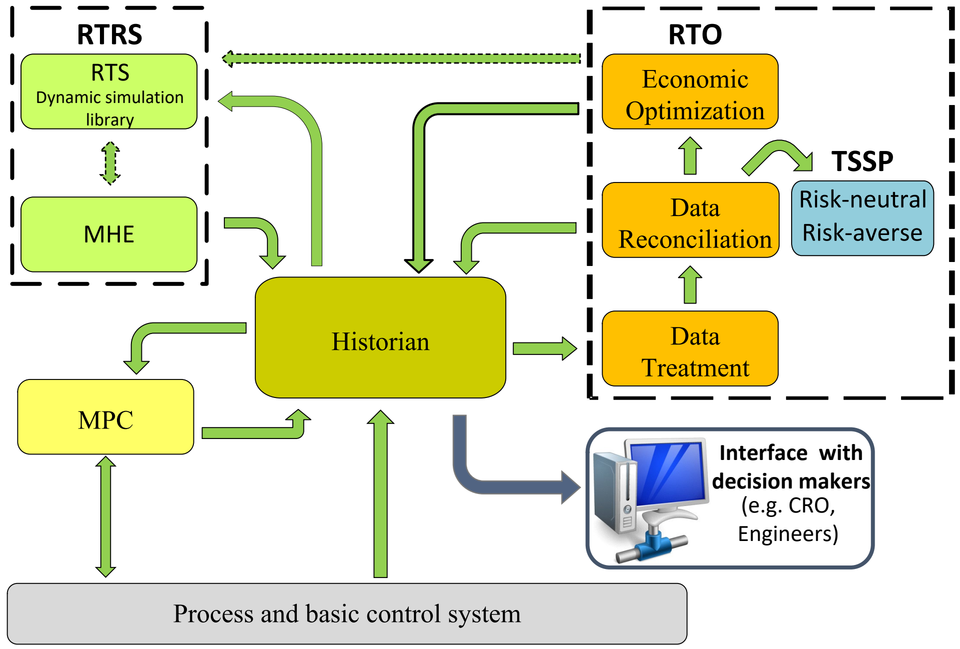


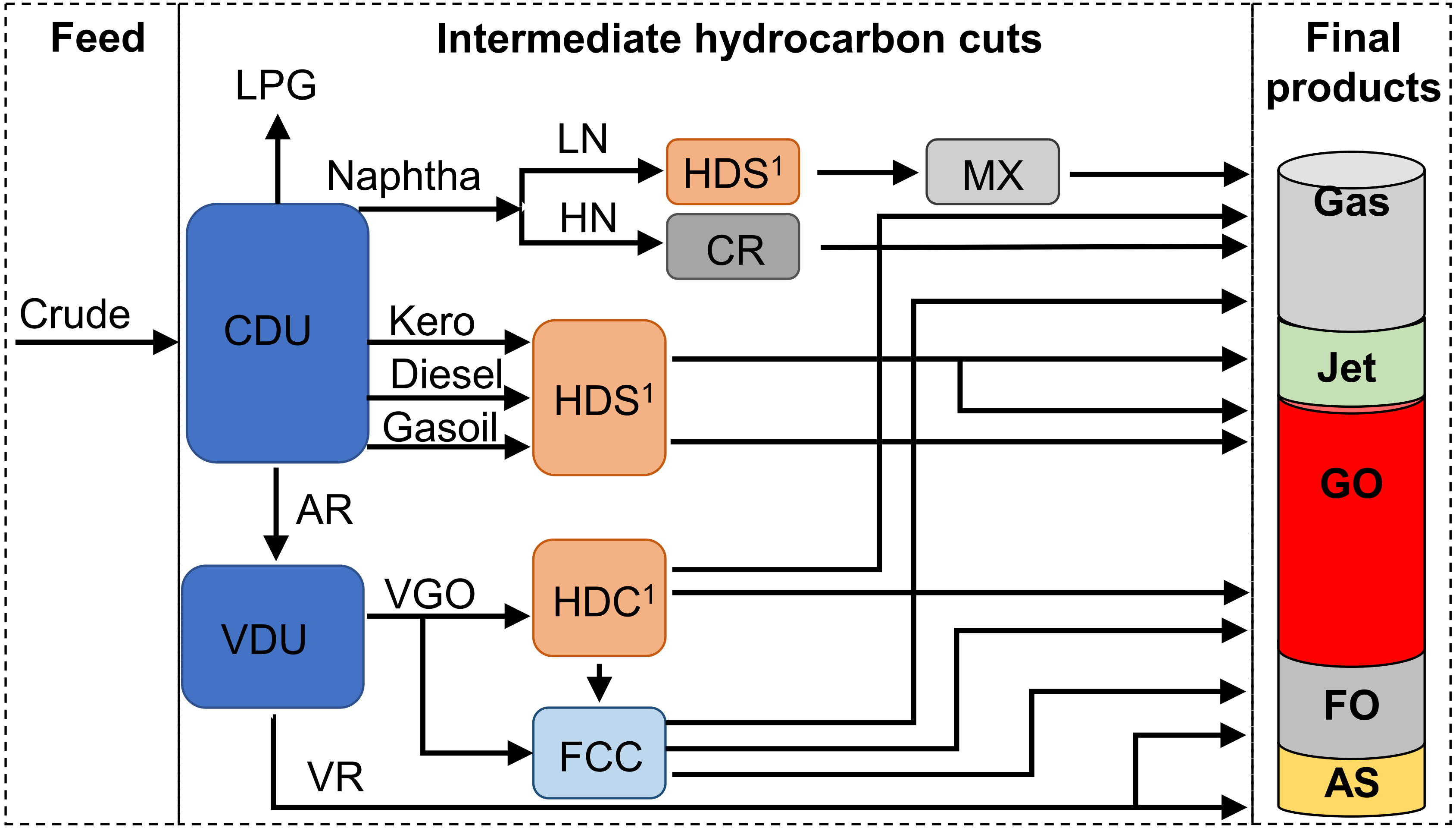
4400 variables
4700 equations

8371 variables
7789 equations

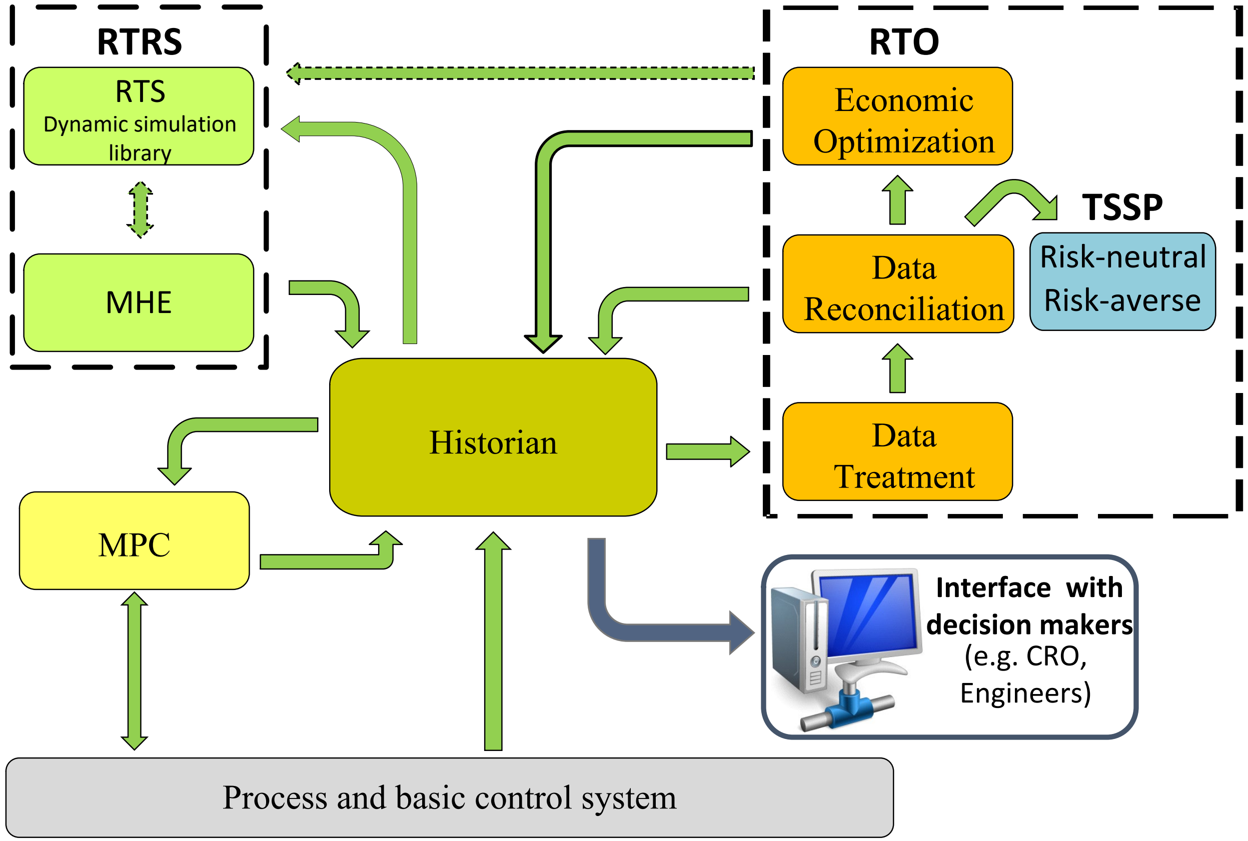
Conclusions

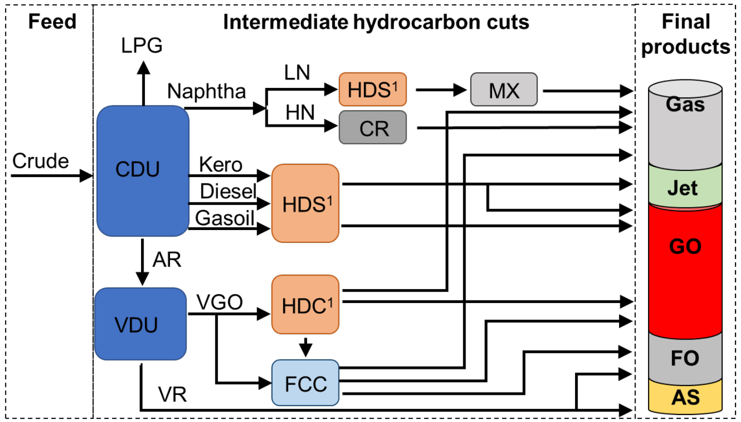
- Dificultad para mantener modelos
  - Parámetros, estados, etc.
  - Cambios en la estructura de la planta
- Especificar grados de libertad
- Interfaces Inteligentes





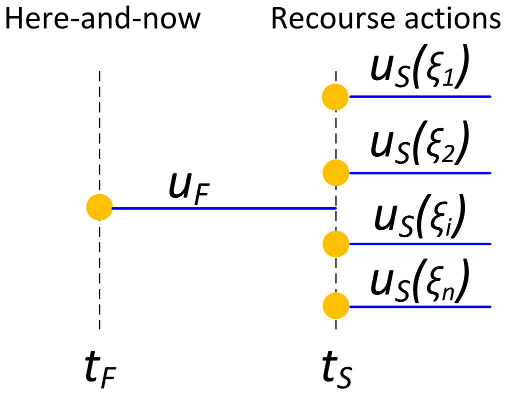
- Crude oil changes every 2-3 days
- Uncertain properties of new feeds impact downstream during changeover periods
- H_2 demand is directly affected by feed chemical properties (mostly unknown)





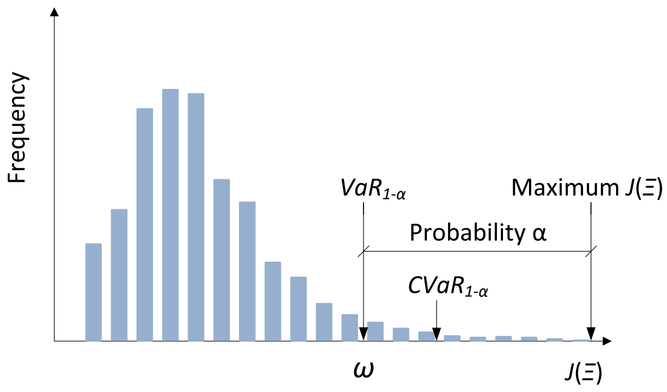
- Crude oil changes every 2-3 days
- Uncertain properties of new feeds impact H_2 demand

Two-stage stochastic programming



Main assumptions:

- H_2 Producers are decided at first stage
- Rest of the variables (e.g. HC loads) are used for recourse once the uncertainty is realized.
- H_2 demand for each process unit is uncertain, responding to a discrete probability function
- 9 scenarios are represented (j = 1…9)



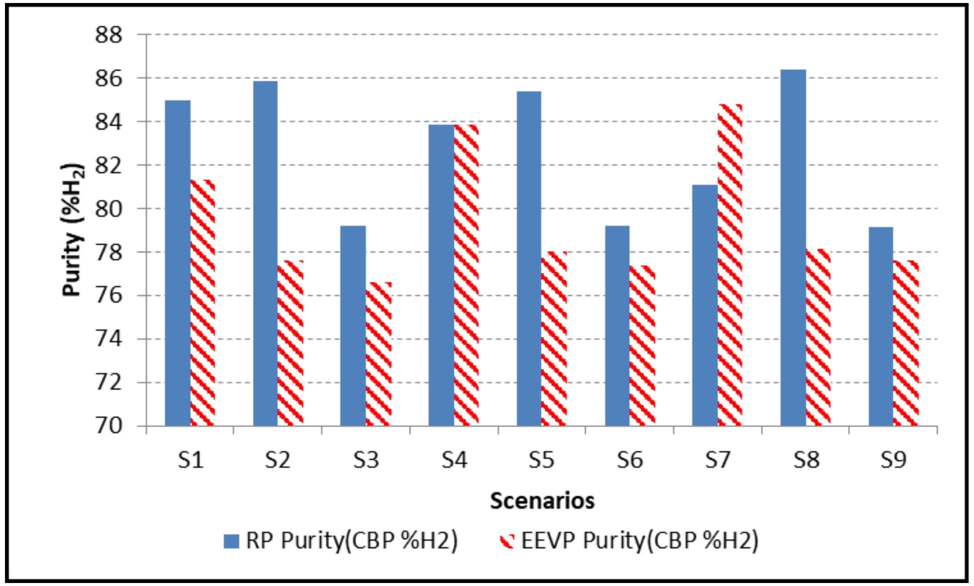
$$\max_{F_{H_2 i}, HC_k(\xi_j), R_k(\xi_j)} J_F\left(-\sum_{i=1}^{2} p_{H_2 i}\cdot F_{H_2 i}\right) + \mathbb{E}\left\{J_S\left(\sum_{k=1}^{4} p_{HC_k}\cdot HC_k(\xi_j) - p_{R_k}\cdot R_k(\xi_j)\right)\right\}$$

s.t.

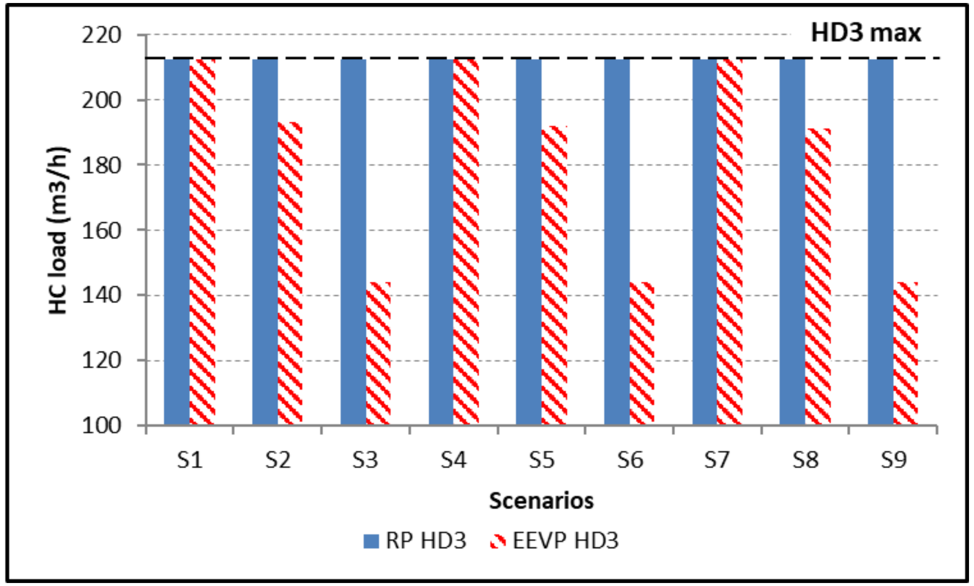
$$h_F(x_F, u_F) = 0,$$
$$g_F(x_F, u_F) \leq 0,$$
$$h_S(x_F, u_F, u_S(\xi), x_S(\xi)) = 0 \quad \forall \xi \in \Xi,$$
$$g_S\big(x_F, u_F, x_S(\xi), u_S(\xi)\big) \leq 0 \quad \forall \xi \in \Xi,$$

Two-stage stochastic problem

Petronor case study – Risk-neutral



Low purity header hydrogen purity at scenarios S1 to S9 applying RP and EEVP



RP and EEVP solutions for HC loads of process unit HD3